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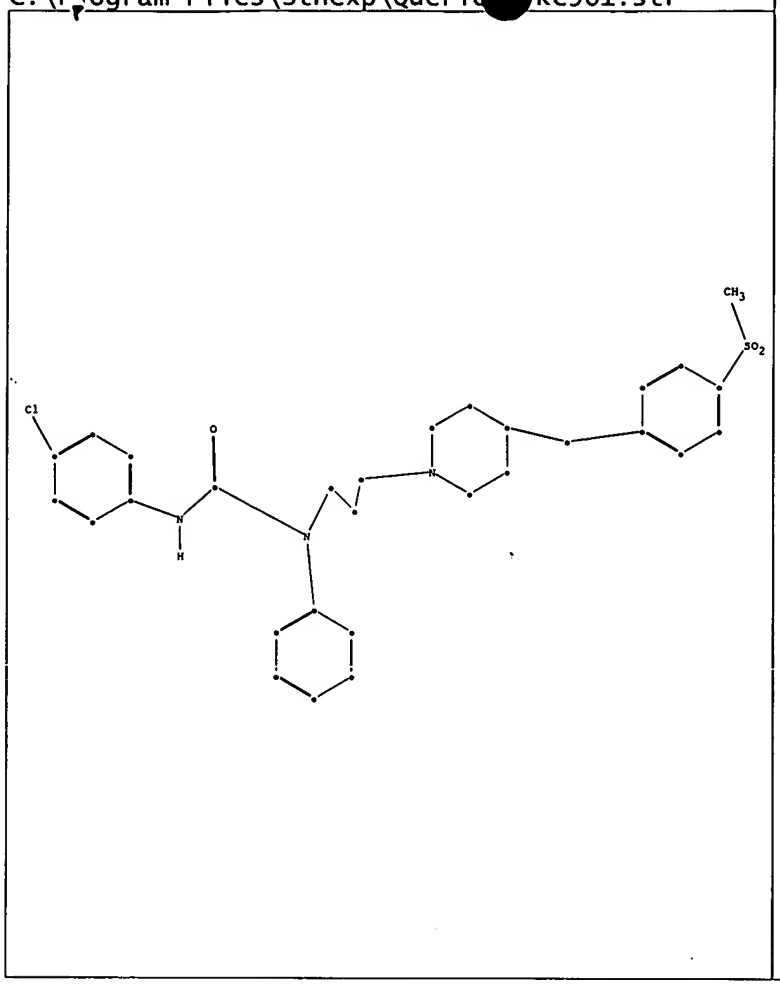
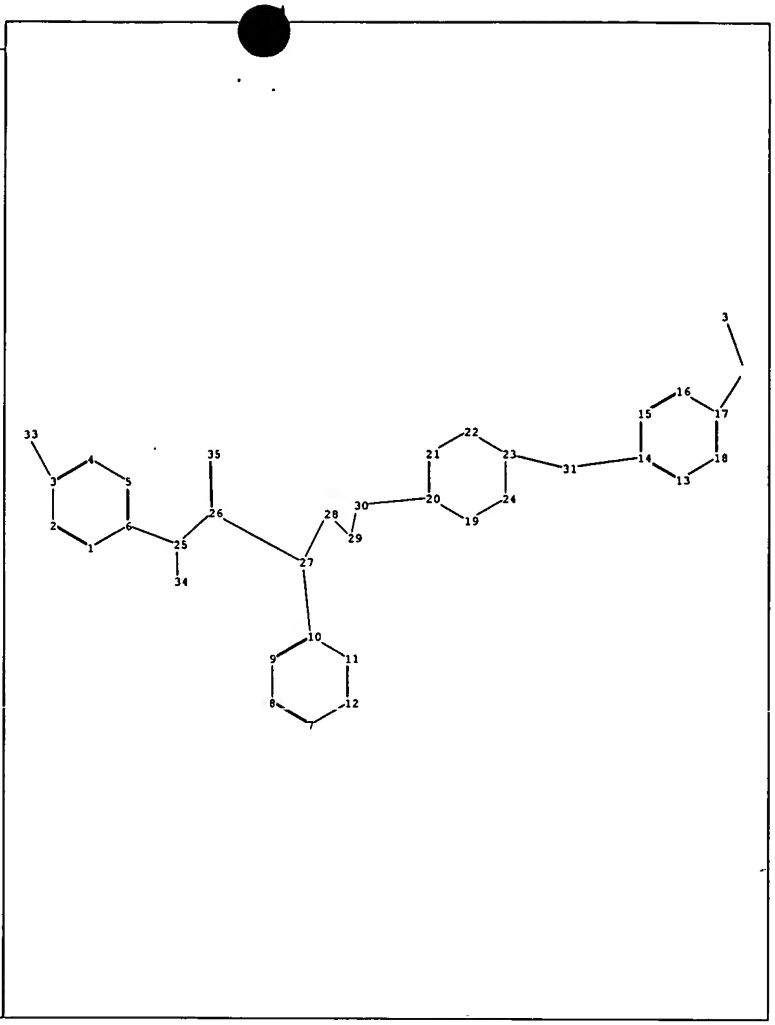




chain nodes :
25 26 27 28 29 30 31 32 33 34 35 36
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
chain bonds :
3-33 6-25 10-27 14-31 17-32 20-30 23-31 25-26 25-34 26-27 26-35 27-28 28-29
29-30 32-36
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15
15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24
exact/norm bonds :
6-25 10-27 19-20 19-24 20-21 20-30 21-22 22-23 23-24 25-26 26-27 26-35 27-28
exact bonds :
3-33 14-31 17-32 23-31 25-34 28-29 29-30 32-36
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15
15-16 16-17 17-18
isolated ring systems :
containing 1 : 7 : 13 : 19 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS

=>
Uploading rkc961.str

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

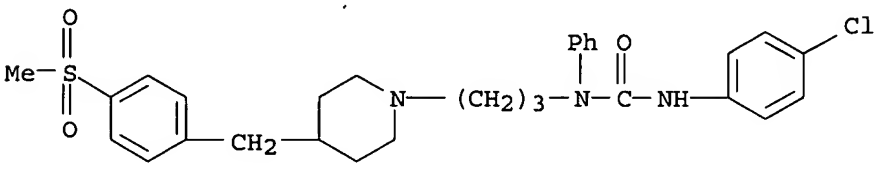
=> s l1 ful
FULL SEARCH INITIATED 09:16:36 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 4 TO ITERATE

100.0% PROCESSED 4 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

L2 2 SEA SSS FUL L1

=> d 1-2

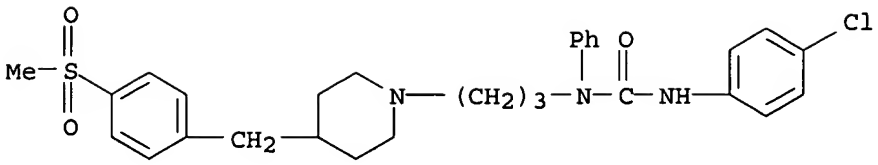
L2 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2003 ACS on STN
RN 333796-51-3 REGISTRY
CN Urea, N'-(4-chlorophenyl)-N-[3-[4-[[4-(methylsulfonyl)phenyl]methyl]-1-piperidinyl]propyl]-N-phenyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C29 H34 Cl N3 O3 S
CI COM
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1947 TO DATE)
1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

L2 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2003 ACS on STN
RN 333796-44-4 REGISTRY
CN Urea, N'-(4-chlorophenyl)-N-[3-[4-[[4-(methylsulfonyl)phenyl]methyl]-1-piperidinyl]propyl]-N-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)
MF C29 H34 Cl N3 O3 S . Cl H
SR CA
LC STN Files: CA, CAPLUS
CRN (333796-51-3)



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1 REFERENCES IN FILE CA (1947 TO DATE)
1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	151.51	151.72

FILE COVERS 1907 - 11 Aug 2003 VOL 139 ISS 7
FILE LAST UPDATED: 10 Aug 2003 (20030810/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l2
L3 1 L2

=> d fbib abs fhitstr

L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2001:265384 CAPLUS
DN 134:280712
TI N-[3-(4-benzylpiperidin-1-yl)propyl]urea compounds, process for producing the same and use thereof for anti-AIDS drugs
IN Kurasawa, Osamu; Imamura, Shinichi; Hashiguchi, Shohei; Nishimura, Osamu; Kanzaki, Naoyuki; Baba, Masanori
PA Takeda Chemical Industries, Ltd., Japan
SO PCT Int. Appl., 90 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001025199	A1	20010412	WO 2000-JP6908	20001004
	W: AE, AG, AL, AM, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CN, CR, CU, CZ, DM, DZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MA, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
				JP 1999-284495 A	19991005
	JP 2001172260	A2	20010626	JP 2000-308006	20001003
				JP 1999-284495 A	19991005
	AU 2000075560	A5	20010510	AU 2000-75560	20001004
				JP 1999-284495 A	19991005
				WO 2000-JP6908 W	20001004
	EP 1219605	A1	20020703	EP 2000-964649	20001004
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
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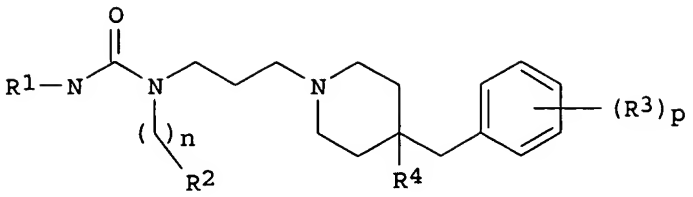
OS MARPAT 134:280712
GI



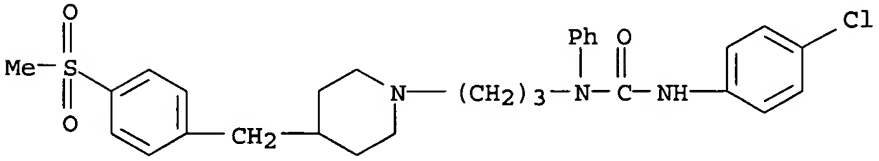
I

AB Compds. represented by general formula (I; wherein R1 represents optionally substituted hydrocarbyl; R2 represents optionally substituted cyclic hydrocarbyl or an optionally substituted heterocycle; R3 represents halogeno, optionally substituted carbamoyl, optionally substituted sulfamoyl, sulfonate-origin acyl, optionally substituted C1-4 alkyl, optionally substituted C1-4 alkoxy, optionally substituted amino, nitro or cyano; R4 represents hydrogen or hydroxy; n is 0 or 1; and p is 0 or an integer of from 1 to 4) or salts thereof, which exhibit an excellent CCR5 (.beta. chemokine receptor) antagonism and are useful as preventives and remedies for HIV infection of human peripheral blood mononuclear cells, in particular, AIDS, are prepd. Thus, a soln. of N-[3-(4-benzyl-1-piperidinyl)propyl]aniline dihydrochloride and Et3N in CH2Cl2 was added dropwise to a soln. of Ph isocyanate in THF at room temp. over 1 h and stirred at room temp. for 12 h to give N-[3-(4-benzyl-1-piperidinyl)propyl]-N-phenyl-N'-phenylurea hydrochloride (II). II and N-[3-(4-benzyl-1-piperidinyl)propyl]-N'-(4-chlorophenyl)-N-(4-methylphenyl)urea hydrochloride (III) inhibited the binding of [125I]-TANTES to CHO cells expressing human CCR5 by 96 and 100%, rep., at 1.0 .mu.M. A capsule formulation contg. II and a tablet formulation contg. III were prepd.

IT **333796-44-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of [(benzylpiperidinyl)propyl]urea compds. as antagonists of .beta. chemokine receptor and anti-AIDS drugs)

RN 333796-44-4 CAPLUS

CN Urea, N'-(4-chlorophenyl)-N-[3-[4-[[4-(methylsulfonyl)phenyl]methyl]-1-piperidinyl]propyl]-N-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



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RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT